Introduction to Hubbard Model and Exact Diagonalization

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Hubbard model is an important model in theory of strongly correlated electron systems. In this contribution we introduce this model along with numerically exact method of diagonalization of the model.

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I. INTRODUCTION

Hubbard model[1] and its variants constitute an important research topic in theoretical condensed matter physics, particularly in the context of strongly correlated electron systems. Most of the many-body techniques commonly used in condensed matter physics can be learnt in this context. Also there are some theoretical tools and concepts which apply to this model only.

There are already some monographs[2,3], which can be used by experts, along with some text books[4,5,6] which can be consulted for further details of the various methods. In this contribution our aim is to provide a smooth introduction to the model and exact diagonalization technique used in dealing with Hubbard model. This work is based on the set of lectures given by the author in the first IUT school[15] on strongly correlated electron systems.

Analytical methods of solving the Hubbard model are all approximate, except in 1D, where the so called **Bethe ansatz** provides an exact solution[7]. On the other hand there are exact numerical techniques, which are however, either computer time expensive or memory expensive. Therefore one is limited to rather small cluster sizes.

A popular method to solve Hubbard model and many other models in condensed matter physics is **exact diagonalization** (ED) of the models for small clusters which we will study at length in this set of lectures. We encourage the reader to implement the method presented here in a simple `fortran` program. In numerically exact diagonalization method one gets the 'exact' results at a high price, namely limitation to very small cluster sizes (about 18 sites for Hubbard model at half filling), which is essentially due to limited amount of computer RAM one can typically have. If one accepts some error bars in numerical results (which can however be systematically improved), then a family of the so called **Monte Carlo** methods are methods of choice[8]. These methods are essentially exact. The accuracy of the results depends on how much computer time one would likes to spend. In this sense, these family of methods are time expensive, while ED is memory expensive.

One of the important methods to deal with almost any model is Mean Field Theory (MFT). MFT ignores quantum fluctuations; hence becoming less accurate in lower spatial dimensions. Despite this, mean field treatment reveals the wealth of various condensed matter phases can emerge from a simple Hubbard model[4]. In MFT one ignores both spatial and temporal fluctuations. It is possible to retain the temporal fluctuations by performing a full fledged quantum dynamics of the problem. This is the subject of the so called **'dynamical' mean field theory** (DMFT)[9].

There are also a class of approximate analytic methods known as **auxiliary particle** or **slave particle** methods, which are invented to deal with the large U limit of the Hubbard model[10]. This type of techniques are related to the so called **Gutzwiller projection** which are devised to obtain approximate ground state of the Hubbard model at half filling. Generalization of this method to deal with excited states is also there in the market[11].

In the limit of large U, the charge fluctuations in the Hubbard model are frozen and only the spin of electrons can fluctuate. Thereby reducing the physics of the Hubbard model to spin physics described by the so called t-J Model[4].

II. HUBBARD MODEL

A. Non-interacting electrons

The Hamiltonian of a system of non-interacting fermions on a lattice of L sites labeled by i, j, etc can be represented in second quantization by

$$H_0 = \sum_{ij} t_{ij} c_i^\dagger c_j$$

where $c_j^\dagger (c_j)$ creates (annihilates) a fermion in a single-particle orbital ϕ_j localized at site j. In condensed matter applications one can assume ϕ_j's to be Wannier wave functions (Fourier transform of Bloch orbitals). Fermionic operators satisfy the *anti-commutation* relations,

$$\{c_i^\dagger, c_j\} = \delta_{ij}, \quad \text{others} = 0. \tag{1}$$

The coefficients t_{ij} characterize the single-particle matrix elements

$$
\begin{aligned}
t_{ij} &= \langle \phi_i | \left(-\frac{\hbar^2 \nabla^2}{2m} + \hat{v} \right) | \phi_j \rangle \\
&= \int dx \phi_i(x) \left(-\frac{\hbar^2 \nabla^2}{2m} + v(x) \right) \phi_j(x) \tag{2}
\end{aligned}
$$

For many practical purposes it suffices to assume that t_{ij} is none-zero, only when i, j are nearest neighbors in which case it is usually denoted by $-t$, so that the Hamiltonian written in manifestly hermitian format becomes

$$H_0 = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + c_j^\dagger c_i \qquad (3)$$

Assuming the periodic boundary conditions (PBC), the Hamiltonian of the system will be invariant under translation. The irreducible representations of the translation group (due to abelian structure of the group), are one-dimensional (i.e. numbers of type $e^{i\theta}$). Hence the one-particle (or non-interacting=free) Hamiltonian (3) can be diagonalized by a Fourier transformation ($\theta \leftrightarrow kj$)

$$c_k^\dagger = \frac{1}{\sqrt{L}} \sum_j e^{ikj} c_j^\dagger, \qquad (4)$$

Then the Hamiltonian in $|\phi_k\rangle$ basis becomes

$$H_0 = \sum_k \varepsilon_k c_k^\dagger c_k, \quad \varepsilon_k = -2t \cos k, \qquad (5)$$

where ε_k determines a cosine dispersion and represents a band structure with L allowed k values in the first Brillouin zone. Of course a simple cosine may not be a good approximation of the realistic band structure of solids (spaghetti plots). To mimic the realistic band structures, one can add further neighbors' hoppings which generate higher harmonics of the simple cosine band.

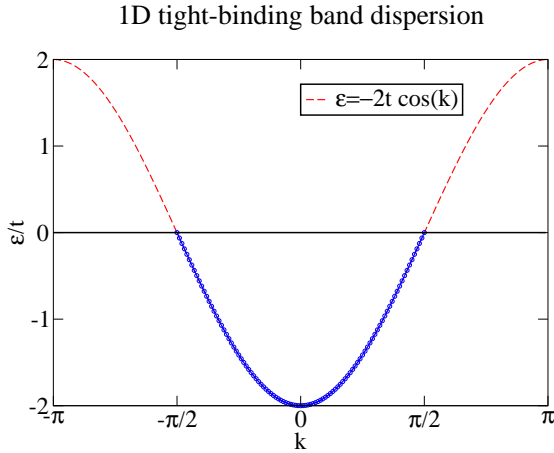### 1D tight-binding band dispersion

FIG. 1: A tight-binding band dispersion in 1D with electron-like Fermi surface.

If the number N of the electrons is equal to number L of the sites, then each allowed k state can be occupied by two $\uparrow$ and $\downarrow$ spins. Hence the ground state of H_0 is constructed by filling the lower half ($\varepsilon_k < 0$) of the band dispersion of Fig. 1 which is denoted by circles on the figure. Since half of the band is filled, the $N = L$ situation is called *half-filling*[16]. This state is known as a Fermi sea

state, usually denoted by $|\text{FS}\rangle$. Second quantized representation of this state is:

$$|\text{FS}\rangle = \prod_{k<k_F} c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger |0\rangle, \qquad (6)$$

where $|0\rangle$ is vacuum state (empty lattice) and k_F is the largest occupied k value ($\pi/2$ here), known as Fermi wave-vector. This expression in first quantized notation corresponds to an slater determinant. So the ground state of a non-interacting Hamiltonian H_0 is characterized by a single slater determinant.

This state is an eigen state of the Hamiltonian

$$H_0|\text{FS}\rangle = E_0|\text{FS}\rangle, \qquad (7)$$

where E_0 is the total energy given by

$$E_0 = \sum_{|k|<\pi/2,\sigma} \varepsilon_k n_{k\sigma} = \int_{-\pi/2}^{\pi/2} \frac{dk}{2\pi} 2 \times (-2t \cos k), \qquad (8)$$

where the single-particle energy summation is carried out over the occupied k states of Fig. 1 shown by circles. Obviously the depicted state has the lowest energy, since the k states have been filled such that lower energy single-particle states are filled first. In this spirit and excited state is create as follows: leave on state k with $|k| < \pi/2$ empty, promoting its electron to another state $k+q$ such that $|k + q| > \pi/2$. This excited with a hole left behind in state k and an electron created in state $k+q$ with, say $\uparrow$ spin is called a 'particle-hole' excitation:

$$H_0|\psi_n\rangle = H_0 c_{k+q\uparrow}^\dagger c_{k\uparrow} |\text{FS}\rangle = \varepsilon_{k,q}^{\text{ph}} |\psi_n\rangle \qquad (9)$$

which is again an eigen state of H_0 with energy $\varepsilon_k^{\text{ph}}(q) = \varepsilon_{k+q} - \varepsilon_k$. This excitation carries a center of mass momentum q. The above discussion can be straightforwardly generalized to higher dimensions.

Evidently the half-filled state $|\text{FS}\rangle$ characterizes a metal, as the energy of the particle-hole excitation can be made arbitrarily small. The above band picture always gives a metal for an odd (in this case one) number of electrons per unit cell. However, as we will argue in the following, there might be situations in which this simple prediction of the band theory fails drastically.

B. Electron-electron interaction

When we have only H_0 (Eq. 3) in the Hamiltonian, then the minimization of energy is achieved by filling the k states *independently* with electrons of opposite spins. Such k space picture in real space translates to equal probabilities $p = 1/4$ for four possible occupation of a single site:

$$\bigcirc \quad \textcircled{\uparrow} \quad \textcircled{\downarrow} \quad \textcircled{\uparrow\downarrow} \qquad (10)$$

The most general form of interaction in second quantization representation which can be added to H_0 is of the form

$$V = \frac{1}{2} \sum_{\mu\nu\alpha\beta} V_{\mu\nu\beta\alpha} c_\mu^\dagger c_\nu^\dagger c_\alpha c_\beta \qquad (11)$$

where $\alpha = \{\alpha, i\}$ is a collective name for the site index i, and spin index σ the two-particle matrix elements is given by

$$V_{\mu\nu\beta\alpha} = \int dx dx' \psi_\mu^*(x) \psi_\nu^*(x') V(|x - x'|) \psi_\beta(x) \psi_\alpha(x')$$
$$(12)$$

usually in metals with appreciable density of states $D(\epsilon_F)$ at the Fermi level, the Coulomb potential $V(|x - x'| = r)$ is screened and obtains the form

$$V(r) = \frac{e^{-r k_{\mathrm{TF}}}}{r}, \qquad (13)$$

where k_{TF}^{-1} is the so called screening length. For the d electron systems where the overlap between the atomic wave functions is small (smaller t), one has narrower band which is synonymous to larger DOS at the Fermi level the screening length is usually on the scale of the Bohr radius a_B^0. Therefore the most important term among all possible $\mu\nu\beta\alpha$ matrix elements is when all the indices correspond to the same site j. In such case, the Pauli principle forces $\mu = \alpha = \uparrow$ and $\beta = \nu = \downarrow$. Denoting the corresponding matrix element with $-2U$ one gets for the screened interaction

$$V = -U \sum_j c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{j\uparrow} c_{j\downarrow} = U \sum_j n_{j\uparrow} n_{j\downarrow}. \qquad (14)$$

If we add this term to H_0, we obtain the celebrated *Hubbard model*

$$H = -t \sum_{\langle i,j \rangle \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_j n_{j\uparrow} n_{j\downarrow}. \qquad (15)$$

For the Hamiltonian in $U \to \infty$ limit the doubly occupied configuration of a single site in Eq. (10) is going to cost a large energy $U n_{j\uparrow} n_{j\downarrow} = U(1)(1)$ for each doubly occupied site. Therefore presence of such term violates the equi-probability of four possible states of a single-site, thereby inducing some kind of correlation by minimizing the double occupancy. Therefore at half-filling, and for large U the ground state charge distribution adjust itself to avoid doubly occupied sites as much as possible; i.e. each site is occupied by a single electron, and that moreover, large value of U makes charge fluctuations around $n_{j\sigma} = 1$ configuration very expensive. Therefore charge fluctuations are frozen and one has an insulator known as *Mott insulator*.

For finite values of U, the two terms of the Hamiltonian (15) compete with each other. The kinetic energy term (corresponding to $U = 0$) tends to delocalize electrons by putting individual electrons in Bloch states.

This limit known as band limit always describes a metal. The U term on the other hand increases the cost of charge fluctuation, leading to an insulator in the opposite limit $U \to \infty$. Therefore there must be a critical value U_c of the order of band width $W = 2zt$ (where z is the coordination number), beyond which one has an insulator. This (first oder at zero temperature) phase transition is known as Mott metal-insulator transition (MIT). The only technique which can handle this model at arbitrary values of U and for arbitrary filling is ED, which will be described in next section.

III. EXACT DIAGONALIZATION

The easiest way to describe the essence of this method is by the example of a two-site Hubbard model. This toy model consists in two sites labeled $0, 1$. In this case the Hubbard model written explicitly (in units in which $t = 1$) reads:

$$\begin{aligned} H &= H_t + H_U \\ &= -\left(c_{0\uparrow}^\dagger c_{1\uparrow} + c_{1\uparrow}^\dagger c_{0\uparrow} + c_{0\downarrow}^\dagger c_{1\downarrow} + c_{1\downarrow}^\dagger c_{0\downarrow} \right) \\ &\quad + U \left(n_{0\uparrow} n_{0\downarrow} + n_{1\uparrow} n_{1\downarrow} \right) \end{aligned} \qquad (16)$$

where sites are labeled as follows:

$$\underbrace{\Box}_{1} \underbrace{\Box}_{0}$$
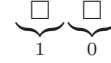
where the site index increases from right to left.

A. Organizing the Hilbert space

To organize the Fock space for this Hamiltonian, one first notes that the number operator $N = \sum_{j\sigma} n_{j\sigma}$ commutes with the Hamiltonian. Therefore one can consider only Hilbert space corresponding to a fixed value of N. Let us consider $N = 2$ for this toy model which corresponds to half-filling condition. The next question arises with regard to the total spin of the electrons: whether they are $\uparrow\uparrow$, $\downarrow\downarrow$ or $\uparrow\downarrow$? First two cases represent triplet state, while the last one corresponds to $S = 0$ (more precisely ($\uparrow\downarrow - \downarrow\uparrow$) is a singlet). Formally it can be checked that the total $S_z = 1/2 \sum_j (n_{j\uparrow} - n_{j\downarrow})$ also commutes with the Hamiltonian and hence a conserved quantity. Therefore there would be no matrix element of the Hamiltonian connecting sections of the Hamiltonian with different values of S_z. The structure of the Hamiltonian will be block diagonal where each block corresponds to a fixed value of S_z. To see this block-diagonal structure, we confine ourselves to $N = 2$ with both triplet and singlet spins.

In sector with quantum numbers $N = 2$ and $S_z = 0$, Hilbert space is six dimensional with six possible basis

states $|\phi_J\rangle$ with $J = 1\ldots6$.

	beginner	expert	computer			
J	algebraic	picture	binary	$I_\downarrow$	$I_\uparrow$	I
1	$c^\dagger_{1\uparrow}c^\dagger_{0\uparrow}|\rangle$	↑ ↑	$|00\rangle_\downarrow|11\rangle_\uparrow$	0	3	3
2	$c^\dagger_{0\downarrow}c^\dagger_{0\uparrow}|\rangle$	○ ↑↓	$|01\rangle_\downarrow|01\rangle_\uparrow$	1	1	5
3	$c^\dagger_{0\downarrow}c^\dagger_{1\uparrow}|\rangle$	↑ ↓	$|01\rangle_\downarrow|10\rangle_\uparrow$	1	2	6
4	$c^\dagger_{1\downarrow}c^\dagger_{0\uparrow}|\rangle$	↓ ↑	$|10\rangle_\downarrow|01\rangle_\uparrow$	2	1	9
5	$c^\dagger_{1\downarrow}c^\dagger_{1\uparrow}|\rangle$	↑↓ ○	$|10\rangle_\downarrow|10\rangle_\uparrow$	2	2	10
6	$c^\dagger_{0\downarrow}c^\dagger_{1\downarrow}|\rangle$	↓ ↓	$|11\rangle_\downarrow|00\rangle_\uparrow$	3	0	12

$$(17)$$

First row indicates three major sets of columns:

- The second column labeled 'beginner' is a way a beginner would define and work with a set of 6 basis states $|\phi_1\rangle$ to $|\phi_6\rangle$.

- The third column labeled 'expert' is a way an expert works with these basis states.

- Columns number 4 to 7 are related to the way a computer organizes and works with the basis states.

Explanation of each columns is as follows:

1. In the first column there is an integer $J = 1\ldots6$ which labels the basis states in the Hilbert space.

2. Second column shows how to obtain the configuration depicted in third column by acting with creation operators on the vacuum $|\rangle$. As an example look at the first basis $|\phi_1\rangle$: Physically, it describes two ↑ electrons in sites number $0, 1$. Therefore we have two choices:

$$|\phi_1^a\rangle = c^\dagger_{1\uparrow}c^\dagger_{0\uparrow}\,|\rangle, \quad \text{or} \quad |\phi_1^b\rangle = c^\dagger_{0\uparrow}c^\dagger_{1\uparrow}\,|\rangle.$$

These two choices by Fermionic anti commutation relations are negative of each other: $|\phi_1^a\rangle = -|\phi_1^b\rangle$. Then the question is: which one is correct way of representing $|\phi_1\rangle$? The answer is that, both of them are fine, the same way one can describe ordinary 3 dimensional vector space with basis $\hat{e}_1 = \hat{x}, \hat{e}_2 = \hat{y}, \hat{e}_3 = \hat{z}$, or say, $\hat{e}_1 = -\hat{x}, \hat{e}_2 = \hat{y}, \hat{e}_3 = \hat{z}$. The important point is to stick to one convention during the entire matrix and vector manipulations. For example, to construct the above table we choose the following convention: (i) ↑ *spin operators sit to the right of ↓ spins.* (ii) *The order of site indices increases from right to left.*

3. Third column is a pictorial representation of the basis vector in real space. We will learn in the following how to work with this intuitive representation of the basis states.

4. The fourth column represents the states as direct product of spin-↓ with spin-↑ state states, where the occupations in up and down spin sectors are represented by sequence of $0, 1$ bits giving rise to a binary representation of the basis states.

For models like, Hubbard model where ↑ and ↓ spins do not admix, this separation makes a good sense. To see this, consider the effect of a term like $c^\dagger_{i\uparrow}c_{j\uparrow}$ on a typical state

$$
\begin{aligned}
|\phi\rangle &= [c^\dagger_{i_1\downarrow}\ldots c^\dagger_{i_N\downarrow}]\,[c^\dagger_{j_1\uparrow}\ldots c^\dagger_{j_M\uparrow}]|\rangle \\
&= [c^\dagger_{i_1\downarrow}\ldots c^\dagger_{i_N\downarrow}]|\rangle_\downarrow\,[c^\dagger_{j_1\uparrow}\ldots c^\dagger_{j_M\uparrow}]|\rangle_\uparrow \\
&=: |\phi_\downarrow\rangle|\phi_\uparrow\rangle,
\end{aligned}
$$

which can be written as

$$
\begin{aligned}
c^\dagger_{i\uparrow}c_{j\uparrow}|\phi_\downarrow\rangle|\phi_\uparrow\rangle &= c^\dagger_{i\uparrow}c_{j\uparrow}[c^\dagger_{i_1\downarrow}\ldots c^\dagger_{i_N\downarrow}][c^\dagger_{j_1\uparrow}\ldots c^\dagger_{j_M\uparrow}]|\rangle \\
&= [c^\dagger_{i_1\downarrow}\ldots c^\dagger_{i_N\downarrow}]\,(-1)^N(-1)^N c^\dagger_{i\uparrow}c_{j\uparrow}[c^\dagger_{j_1\uparrow}\ldots c^\dagger_{j_M\uparrow}]|\rangle \\
&= |\phi_\downarrow\rangle\,c^\dagger_{i\uparrow}c_{j\uparrow}|\phi_\uparrow\rangle.
\end{aligned}
\tag{18}
$$

Here two $(-1)^N$ factors arise from moving each of the $c^\dagger_\uparrow$ operators through a length N sequence of $c^\dagger_\downarrow$ operators. Therefore, *when operating in spin-↑ sector, we need not worry about spin-↓ configuration and vice versa.*

5. The last three column indicate the way a computer understands and stores these basis state. There is only one integer I stored on computer which fully represents the occupation pattern of the ↑ and ↓ electrons when transformed to binary representation of fourth column in Eq. (17). Given I, one can obviously find out $I_\uparrow$ and $I_\downarrow$ through the relation

$$I = 2^L I_\downarrow + I_\uparrow \tag{19}$$

and vice versa. First and last columns of (17) do actually tabulates an array $I = T(J)$ which for any given J, returns the corresponding I. The value of I fully specifies the state. One therefore only to extract the bits of I and find a way to work with bits of integer I.

There remains only a final note on how we have labeled the states. We have labeled the configuration represented by $I = 9$ as fourth ($J = 4$) basis vector, etc. We could have labeled them in any order, so that $I = 9$ would have corresponded to, e.g. first ($J = 1$) basis vector. The above convention which was suggested by Lin and coworkers[13], has the advantage that the table T can be searched given a value for I in a fast way in order to find out corresponding J value. The essential idea of this convention is the following[13]: For any sector you are interested in, just choose the labels J in such a way that when the above table T is constructed, the I values are ascending function of J.

B. Acting with operators on the basis states

If the action of an operator on a complete basis set is known, then the operator is completely specified.

Eq. (16) has two type of terms: H_U and H_t. When H_U acts on a basis states, it gives non zero contribution for each site j in which both $n_{j\uparrow}$ and $n_{j\downarrow}$ are 1. Therefore the effect of H_U on any basis state gives the same state multiplied by the number of doubly occupied sites $\times U$. Hence the effect of H_U on $|\phi_i\rangle$, $i = 1, 3, 4, 6$ is zero and on $|\phi_2\rangle$ and $|\phi_5\rangle$ is just U. The H_U part is diagonal in occupation number representation:

$$H_U \doteq U \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (20)$$

Now let us concentrate on the effect of H_t on our basis states. Consider, e.g. the sate $|\phi_2\rangle$. H_t in Eq. (16) has 4 terms. But only 2 of them give non zero contribution when they act on $|\phi_2\rangle$: The one which allows an $\uparrow$ spin to hop from site 0 to 1, i.e. $c_{1\uparrow}^\dagger c_{0\uparrow}$, and another one which allows the $\downarrow$ spin at site 0 to jump to site 1, i.e. $c_{1\downarrow}^\dagger c_{0\downarrow}$.

$$H_t|\phi_0\rangle = -t \left(c_{1\uparrow}^\dagger c_{0\uparrow} + c_{1\downarrow}^\dagger c_{0\downarrow} \right) c_{0\downarrow}^\dagger c_{0\uparrow}^\dagger |\rangle$$

$$= -t \left(c_{1\uparrow}^\dagger \overbrace{c_{0\uparrow}}^{\rightarrow} c_{0\downarrow}^\dagger c_{0\uparrow}^\dagger + c_{1\downarrow}^\dagger c_{0\downarrow} c_{0\downarrow}^\dagger \overbrace{c_{0\uparrow}^\dagger}^{\leftarrow} \right) |\rangle$$

$$= -t \left(-c_{1\uparrow}^\dagger c_{0\downarrow}^\dagger c_{0\uparrow} c_{0\uparrow}^\dagger |\rangle + c_{1\downarrow}^\dagger c_{0\uparrow}^\dagger c_{0\downarrow} c_{0\downarrow}^\dagger |\rangle \right)$$

$$= -t \left(-c_{1\uparrow}^\dagger c_{0\downarrow}^\dagger |\rangle + c_{1\downarrow}^\dagger c_{0\uparrow}^\dagger |\rangle \right)$$

where in the third line we have used the Fermionic anti-commutation relations with associated minus signs needed for each exchange of Fermionic operators with different indices. Also in the last step we have used the fact that $c_{j\sigma} c_{j\sigma}^\dagger |\rangle = (1 - n_{j\sigma})|\rangle = |\rangle$, as the vacuum state $|\rangle$ contains no particles. Rearranging the Fermionic operators to comply with our convention we get

$$H_t|\phi_2\rangle = -t \left(+|\phi_3\rangle + |\phi_4\rangle \right). \quad (21)$$

This way of working with commutations and algebra is not a convenient for putting on computers. As we already showed in Eq. (18), the up and down spins hop separately. Therefore, when an spin $\uparrow$ electron hops from site say j to site i, one only needs to count a (-1) factor for each $\uparrow$ spin electron over which it passes. Since when $c_{j\uparrow}$ has to moved through a chain of $c_{j'\uparrow}^\dagger$ operators with $j' \neq j$, until it reaches $c_{j\uparrow}^\dagger$, there they form a $(1 - n_{j\uparrow})$ operator which commutes with all other remaining $c_{j''\uparrow}^\dagger$ operators to reach the vacuum $|\rangle$ where it produces $|\rangle$ itself.

With this argument in mind, one can most conveniently work with the pictorial representation of states: The effect of H_t on $|\phi_2\rangle$ is to either move an $\uparrow$ spin to

site 1, or to move a $\downarrow$ spin to site 1. In the former case one gets $(-1)^0 |\phi_3\rangle$ where the exponent 0 is because the $\uparrow$ spin at site 0 passes through no other $\uparrow$ spin when it hops to site 1. Similarly the later case gives $|\phi_4\rangle$. According to the Hamiltonian (16), each of these processes happens with an amplitude $-t$ and thus one can pictorially see that

$$H_t|\phi_2\rangle = -t \left(+|\phi_3\rangle + |\phi_4\rangle \right).$$

With this in mind it is almost trivial to check that

$$H_t|\phi_1\rangle = 0$$
$$H_t|\phi_2\rangle = -t \left(|\phi_3\rangle + |\phi_4\rangle \right)$$
$$H_t|\phi_3\rangle = -t \left(|\phi_2\rangle + |\phi_5\rangle \right)$$
$$H_t|\phi_4\rangle = -t \left(|\phi_2\rangle + |\phi_5\rangle \right)$$
$$H_t|\phi_5\rangle = -t \left(|\phi_3\rangle + |\phi_4\rangle \right)$$
$$H_t|\phi_6\rangle = 0 \quad (22)$$

Therefore in this basis the hopping term has the following matrix representation:

$$H_t \doteq -t \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (23)$$

Therefore the matrix representation of the entire Hamiltonian in this basis becomes

$$H \doteq \left(\begin{array}{c|cccc|c} 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & U & -t & -t & 0 & 0 \\ 0 & -t & 0 & 0 & -t & 0 \\ 0 & -t & 0 & 0 & -t & 0 \\ 0 & 0 & -t & -t & U & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right) \quad (24)$$

Clearly the above block diagonal structure has a parallel with the following form for the S_z matrix:

$$S_z \doteq \left(\begin{array}{c|cccc|c} +1 & & & & & \\ \hline & 0 & & & & \\ & & 0 & & & \\ & & & 0 & & \\ & & & & 0 & \\ \hline & & & & & -1 \end{array} \right) \quad (25)$$

In other words state $|\phi_1\rangle$ has a quantum number $S_z = +1$, while $|\phi_6\rangle$ has $S_z = -1$. The set of states $|\phi_2\rangle \ldots |\phi_5\rangle$ belong to $S_z = 0$ sector. If we had confined ourselves to $S_z = 0$ sector, we would have obtained a four dimensional Hilbert space in which the Hamiltonian could be represented by the 4×4 block of Eq. (24).

The method described after Eq. (21) has the advantage that for large matrices, precisely the same steps can be taken with a simple computer code that implements the logic described above. When coding the procedure we have the binary representation in column 4 of Eq. (17) in mind for the occupation pattern of $\uparrow$ and $\downarrow$ electrons. But there is only one integer I (7th column) stored on computer the binary representation of which precisely corresponds to column 4. Extracting $I_\uparrow$ and $I_\downarrow$ from a given I in `fortran` is as simple as

```
I_up=mod(I,2**L);  I_dn=I/2**L
```

Most of the standard high level programming languages such as `c++` and `fortran 90` have appropriate intrinsic functions for bitwise operations on integer which are able to access and examine or change individual bits of a given integer p (can be $I_\uparrow$ or $I_\downarrow$). Therefore an integer `I` completely specifies the occupation pattern in each spin sector. For example the Intel Fortran compiler has following commands for bitwise manipulation of an integer `p`

$$
\begin{array}{|l|l|}
\hline
\texttt{IBSET(p,b)} & c_b^\dagger \\
\texttt{IBCLR(p,b)} & c_b \\
\texttt{BTEST(p,b)} & n_b \\
\hline
\end{array}
\quad (26)
$$

For more details please consult the Intel Fortran language manual[14]. Also more implementation notes can be found in Lin et.al.[13].

C. Diagonalization of the matrix: Space symmetries

So far we have made use of the symmetries of the *Hamiltonian* itself to reduce the dimension of the matrix to be diagonalized. For example conservation of S_z (equivalent to $[S_z, H] = 0$) reduces the 6×6 matrix to two 1×1 (trivial) and one 4×4 matrix. The commutation relation between e.g. S_z and H is quite general, and independent of the geometry of the lattice in use.

Now we would like to make use of the spatial symmetries in order to diagonalize the 4×4 matrix in $S_z = 0$ sector manually. For a two site problem composed of sites $0, 1$, there is a mirror reflection operator M which has the following action on real lattice:

$$M(0) = 1, \quad M(1) = 0 \quad (27)$$

Corresponding to operation M which is a member of spatial symmetry group of the underlying lattice, there is an operator $\mathcal{M}$ in Hilbert space which acts on the state vectors. For example consider the effect of $\mathcal{M}$ on state $|\phi_3\rangle$ which reads

$$\mathcal{M}c_{0\downarrow}^\dagger c_{1\uparrow}^\dagger |0\rangle = c_{M(0)\downarrow}^\dagger c_{M(1)\uparrow}^\dagger |0\rangle = c_{1\downarrow}^\dagger c_{0\uparrow}^\dagger |0\rangle, \quad (28)$$

or $\mathcal{M}|\phi_3\rangle = |\phi_4\rangle$. Similarly, $\mathcal{M}|\phi_4\rangle = |\phi_3\rangle$, etc. which is

summarized as follows

$$
\begin{aligned}
\mathcal{M}|\phi_1\rangle &= -|\phi_1\rangle \\
\mathcal{M}|\phi_2\rangle &= |\phi_5\rangle \\
\mathcal{M}|\phi_3\rangle &= |\phi_4\rangle \\
\mathcal{M}|\phi_4\rangle &= |\phi_3\rangle \\
\mathcal{M}|\phi_5\rangle &= |\phi_2\rangle \\
\mathcal{M}|\phi_6\rangle &= -|\phi_6\rangle
\end{aligned}
$$

The first and last lines of the above equation indicate that states $|\phi_j\rangle$ with $j = 1, 6$ are eigen states of $\mathcal{M}$ (parity operator) with eigen values ± 1. Line numbers 3,4 however, indicate that states $|\phi_3\rangle$ and $|\phi_4\rangle$ do not have definite parity. Instead a new combination $|\phi_\pm\rangle = \frac{1}{\sqrt{2}}(|\phi_3\rangle \pm |\phi_4\rangle)$, has a definite parity: $\mathcal{M}|\phi_\pm\rangle = \pm|\phi_\pm\rangle$. Similarly from $|\phi_2\rangle$ and $|\phi_5\rangle$, symmetric and antisymmetric combinations will have definite parity.

The eigenvalues $\pm$ of parity operator $\mathcal{M}$ partition the Hilbert space into two pieces which belong either to $+1$ eigen value:

$$
\begin{aligned}
\mathcal{M}(|\phi_3\rangle + |\phi_4\rangle) &= +(|\phi_3\rangle + |\phi_4\rangle) \\
\mathcal{M}(|\phi_2\rangle + |\phi_5\rangle) &= +(|\phi_2\rangle + |\phi_5\rangle),
\end{aligned}
\quad (29)
$$

or to -1 eigen value:

$$
\begin{aligned}
\mathcal{M}|\phi_1\rangle &= -|\phi_1\rangle \\
\mathcal{M}|\phi_6\rangle &= -|\phi_6\rangle \\
\mathcal{M}(|\phi_3\rangle - |\phi_4\rangle) &= -(|\phi_3\rangle - |\phi_4\rangle) \\
\mathcal{M}(|\phi_2\rangle - |\phi_5\rangle) &= -(|\phi_2\rangle - |\phi_5\rangle)
\end{aligned}
\quad (30)
$$

If we knew this when finding out the effect of H_t in Eq. (22), we would have acted on the following states:

$$
\begin{aligned}
|\psi_1\rangle &= |\phi_1\rangle \\
|\psi_2\rangle &= (|\phi_2\rangle + |\phi_5\rangle)/\sqrt{2} \\
|\psi_3\rangle &= (|\phi_3\rangle + |\phi_4\rangle)/\sqrt{2} \\
|\psi_4\rangle &= (|\phi_3\rangle - |\phi_4\rangle)/\sqrt{2} \\
|\psi_5\rangle &= (|\phi_2\rangle - |\phi_5\rangle)/\sqrt{2} \\
|\psi_6\rangle &= |\phi_6\rangle
\end{aligned}
\quad (31)
$$

Eq. (31) defines the so called, symmetry adopted basis in which the action of, say, H_t is enormously simplified:

$$
\begin{aligned}
H_t|\psi_1\rangle &= 0 \\
H_t|\psi_2\rangle &= -2t|\psi_3\rangle \\
H_t|\psi_3\rangle &= -2t|\psi_2\rangle \\
H_t|\psi_4\rangle &= 0 \\
H_t|\psi_5\rangle &= 0 \\
H_t|\psi_6\rangle &= 0
\end{aligned}
\quad (32)
$$

Similarly the only none zero matrix elements of H_U are given by:

$$H_U|\psi_2\rangle = U|\psi_2\rangle, \quad H_U|\psi_5\rangle = U|\psi_5\rangle \quad (33)$$

How do we generate a symmetry adopted basis? There is a very powerful theorem in group representation theory which in case of one dimensional representations is easy to implement and reads[12]:

$$\psi^{(p)} = \sum_R \Gamma_p(R)^* R\phi \qquad (34)$$

In this equation ϕ is an arbitrary state to begin with. R is an element of the symmetry group which in this case and be either $\mathcal{I}$ or $\mathcal{M}$. Γ_p is the irreducible representation of the group which for group $\{\mathcal{I}, \mathcal{M}\}$ are numbers ± 1 for even and odd parity. Reader can easily check that feeding $\phi = |\phi_i\rangle$, with $i = 1,\ldots,6$ is going to generate the symmetry adopted basis Eq. (31). Similar technique can be used to generate states with definite $\vec{k}$ values when dealing with problems of translational invariance.

In symmetry adopted basis total Hamiltonian in $S_z = \pm 1$ sectors ($\{|\psi_1\rangle, |\psi_6\rangle\}$ sub-space) remains diagonal with eigen values equal to 0, as it was. In $S_z = 0$ sector it will become:

$$H \doteq \begin{pmatrix} U & -2t & 0 & 0 \\ -2t & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{pmatrix} \qquad (35)$$

In this sector as well, there are one eigen value equal to 0 which corresponding to eigen state $|\psi_4\rangle$. Note that $|\psi_4\rangle$ is the $S_z = 0$ component of a triplet. Therefore the triplet state lies at zero energy:

$$E_t = 0, \quad \text{for triplet state } (S_z = +1, 0, -1) \qquad (36)$$

The fact that $\{|\phi_1\rangle, |\phi_5\rangle, |\phi_6\rangle\}$ form a triplet is consistent with having odd spatial parity in Eq. (30).

The eigen value corresponding to $|\psi_5\rangle$ is U which is always positive and above the triplet $E_t = 0$.

To find out the remaining two eigen values in the $\{|\psi_2\rangle, |\psi_3\rangle\}$ sector, we note that first of all, this sector has even spatial parity, and hence is spin singlet. Hamiltonian is $U/2\mathcal{I} + U/2\sigma_z - 2t\sigma_x$, where σ_x, σ_z are Pauli matrices, and $\mathcal{I}$ is the unit 2×2 matrix, so that the eigenvalues at spin singlet sector become

$$E_s^\pm = U/2 \pm \sqrt{(U/2)^2 + 4t^2} \qquad (37)$$

Therefore the ground state is a singlet with energy E_s^-, while the first excited state is a triplet with $E_t = 0$. Second excited state is $|\psi_5\rangle$, with energy U, and final excited state has energy E_s^+.

IV. STRONG CORRELATIONS AND SPIN PHYSICS

As we already saw in previous section, the ground state of the two site Hubbard model is a singlet with energy $E_s^- = U/2 - \sqrt{U^2/4 + 4t^2}$, The ground state wave function

$$|E_s^-\rangle = 4|\psi_2\rangle + \left(U + \sqrt{U^2 + 16}\right)|\psi_3\rangle \qquad (38)$$

in large U limit is dominated by $|\psi_3\rangle \sim |\phi_3\rangle + |\phi_4\rangle$ in which there is no doubly occupied configuration, and hence charge fluctuations are suppressed.

Since the first excited state is at $E_t = 0$. The splitting between these two states for large $U \gg t$ is:

$$-J = E_s - E_t = U/2 - \sqrt{U^2/4 + 4t^2} \approx -\frac{4t^2}{U} \qquad (39)$$

Therefore the singlet state is slightly below $(-4t^2/U)$ the triplet state. This indicates that in large U limit, the low-energy physics of Hubbard model is given by spin fluctuations which are anti ferromagnetic (singlet has lower energy). This observation in a two site Hubbard model is indeed very general and it can be shown using a unitary transformation that the Hubbard model at large U limit can be mapped into the so called t-J model, where there are AF spin fluctuations along with hoppings restricted to subspace with no double occupancy[4].

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[15] Isfahan University of Technology, June 2007

[16] Note that if fermions to be filled in the band states where spin-less, the band would be completely filled.